

AUTOMATIC IDENTIFICATION OF COMPOUNDS IN A SAMPLE MIXTURE BY MEANS OF NMR SPECTROSCOPY

ABSTRACT OF THE DISCLOSURE

A process for quantitative and qualitative analysis for identifying compounds
5 in a sample mixture involves the identification of a set of reference spectra selected according
to a measured condition of the sample, which collectively define a composite spectrum which
best matches a spectrum produced from the sample. The compounds associated with
respective reference spectra of the identified set are the compounds that are determined to be
likely to be present in the sample. Quantities of the compounds may be determined from the
10 intensities of certain representative peaks associated with the compounds, relative to the
intensity of a peak associated with a reference compound which is unaffected by the
measured condition of the sample. A measured condition may be pH of the sample, for
example, and an accurate measurement of pH can be obtained from the test spectrum. Thus,
given a test spectrum of a sample and given a set of reference spectra, the process can
15 identify and quantify compounds present in the sample. A process for producing reference
spectra as a function of condition factor is also disclosed and a process for automatically pre-
processing a spectrum from an NMR system is disclosed.

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